Ionization of highly charged relativistic ions by neutral atoms and ions

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Ionization of highly charged relativistic ions by neutral atoms and ions is considered. Numerical results of recently developed computer codes based on the relativistic Born and the equivalent-photon approximations are presented. The ionization of the outer shells dominate. For the outer projectile electron shells, which give the main contribution to the process, the non-relativistic Schrödinger wave functions can be used. The formulae for the non-relativistic reduction of the Dirac matrix-elements are obtained for ionization of electrons with arbitrary quantum numbers n and ℓ.

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I. INTRODUCTION

Projectile ionization, also referred to as electron loss or stripping, is an important charge-changing process playing a critical role in many applications such as heavy-ion driven inertial fusion, ion-beam lifetimes in accelerators, medical science, material technology and others (see, e.g., [1] – [3]).

In order to calculate the non-relativistic ionization cross sections for ion-atom collisions a computer code called LOSS was developed using the Born approximation [4] with account for the screening as well as antiscreening effects. Non-relativistic Schrödinger wave functions are used to describe the electronic structure. This is a good approximation for the outer shell electrons, which play the dominant role.

Relativistic ionization has been pioneered at Stanford by Anholt and collaborators [5] and it is reviewed in several books and review articles (see e.g., [6]– [8]). Numerical calculations of relativistic ionization cross sections are presented in the literature mainly for ionization of H- and He-like ions from the ground 1s state (see, e.g., [9] - [15]).

Recently, two new computer codes LOSS-R (Relativistic Loss) and HERION (High Energy Relativistic IONization) have been developed for calculation of the relativistic ionization cross sections. The LOSS-R code [16] was created on the basis of the non-relativistic LOSS code [4] using the relativistic Born approximation in the momentum-transfer representation without magnetic interactions. The HERION code [17] uses the dipole and impulse approximations with relativistic wave functions but it also neglects the magnetic interactions.

It is the aim of the present work to provide a theoretical framework for ionization in relativistic ion-atom collisions with possible account for the magnetic interactions for an arbitrary many-electron ions. The formulae obtained can be used for projectile ions such as U^{28+} colliding with the rest-gas atoms and molecules at energies up to a few GeV/u. Such heavy many-electron ions are of practical implications for the international FAIR project at GSI Darmstadt [18].

In section 2 the main formulae for relativistic ionization are recapitulated, also in order to establish the notation. Numerical results due to the LOSS-R and HERION codes are given in section 3. In section 4 the non-relativistic reduction of the Dirac matrix-elements is done.

II. FIRST ORDER PERTURBATION THEORY OF RELATIVISTIC IONIZATION

An accurate procedure to include the relativistic effects in ionization cross sections using the plane wave Born approximation is given in [6]. There, the cross section summed over the magnetic quantum numbers and presented in the momentum-transfer q-representation is given in the form:

$$\frac{d\sigma}{dE} = 8\pi(Z_T\alpha)^2\left(\frac{c}{v}\right)^2\int_{q_0}^{\infty}\frac{dq}{q^3}(|F(q)|^2 + \frac{\beta^2(1-q_0^2/q^2)}{(1-\beta^2 q_0^2/q^2)^2}|G(q)|^2), \tag{1}$$

where $\alpha = e^2/\hbar c$ denotes the fine-structure constant, Z_T the effective charge of the target atom, $q_0 = \omega/v$, and ω is the ionization energy. The ion velocity is given by the relativistic factor $\beta = v/c$. The matrix-elements F and G are evaluated in a x, y, z coordinate system in which the z-axis lies along the momentum transfer vector $\vec{q}$. The x-axis lies in the plane formed by the vectors $\vec{q}$ and the projectile velocity $\vec{v}$. They contribute incoherently to the cross section due to different selection rules for the final magnetic substates. The matrix elements F and G are given by [6]

$$F(q) \equiv < f|e^{iqz}|i >, \tag{2}$$

$$G(q) \equiv < f|\alpha_x e^{iqz}|i > . \tag{3}$$

where $|i>$ and $|f>$ denote the wave functions in the initial and final states and α_x the x-component of the Dirac matrix vector $\vec{\alpha}$. This is a useful splitting: the F-term tends to a constant for $\gamma \to \infty$ whereas the G-term increases as $ln\gamma$ due to a contribution of the 'equivalent' photons. The matrix element F is the main term in the non-relativistic ionization, e.g. in the formulae of the LOSS code [4] whereas the matrix element G appears for relativistic ionization. The G-term can be calculated numerically if the Dirac wave functions with the large and small components are known.

The equivalent photon approximation can be obtained from eq. (1): Due to the photon pole, the second term will dominate at high energies. For small q-values the quantity $G(q)$ is directly related to the dipole matrix element:

$$G(0) = \frac{m\omega}{\hbar^2} < f|z|i > \equiv \frac{m\omega}{\hbar^2}D_{fi}. \tag{4}$$

The integral over q in eq. (1) has a dominant contribution at $q \sim q_0$. In the integration over q, we may assume that $G(q) = G(q_0)$. Then the integral diverges logarithmically at large q. One can introduce a suitable cutoff q_{max} which corresponds to a cutoff impact parameter b_{min} in the impact-parameter space. In turn, the dipole moment determines the photoionization cross section (see e.g., [19], eq. (69.2)):

$$\sigma(\omega) = \frac{2\pi e^2\hbar^2}{m^2 c\omega}|D_{fi}|^2 \tag{5}$$

So the ion-atom ionization cross section can be expressed via a photoionization cross section and the equivalent-photon number.

The PWBA (Plane-Wave Born Approximation) formalism is also used in the calculation of bound-free pair production in antiproton-nucleus collisions (antihydrogen production) [20] and in heavy ion collisions [21]. Pair production may be viewed as ionization of the negative energy Dirac sea. In the pair production process one has to use Dirac wave functions, rather than the Schrödinger wave functions.

In [17] the dipole approximation was realized as a part of the HERION code where the dipole part of relativistic ionization cross section of the projectile ion in collision with a neutral atom is expressed via photoionization cross section $\sigma(\omega)$ (see [7]):

$$\sigma_{dip}(v) = \int_{\omega_{min}}^{\infty} n(\omega)\sigma(\omega)\frac{d\omega}{\omega}, \tag{6}$$

where ω_{min} denotes the ionization threshold and $n(\omega)$ the equivalent-photon number

$$n(\omega) = \frac{2{Z_T}^2\alpha}{\pi}\left(\frac{c}{v}\right)^2\left[xK_0(x)K_1(x) - \frac{1}{2}(\beta x)^2(K_1^2(x) - K_0^2(x))\right],\ x = \frac{\omega_{min}\, b_{min}}{v\gamma}. \tag{7}$$

where $K_n(x)$ is the McDonald function. The parameter b_{min} is defined by the size of the projectile-ion shell nl from which ionization occurs and is given with a good accuracy by

$$b_{min} \approx \frac{n}{\sqrt{I_{nl}/Ry}}a_0, \tag{8}$$

where $a_0 = 0.53 \times 10^{-8}$ cm is the Bohr radius, I_{nl} denotes the binding energy of the nl shell and $Ry = 13.606$ eV is the Rydberg energy unit.

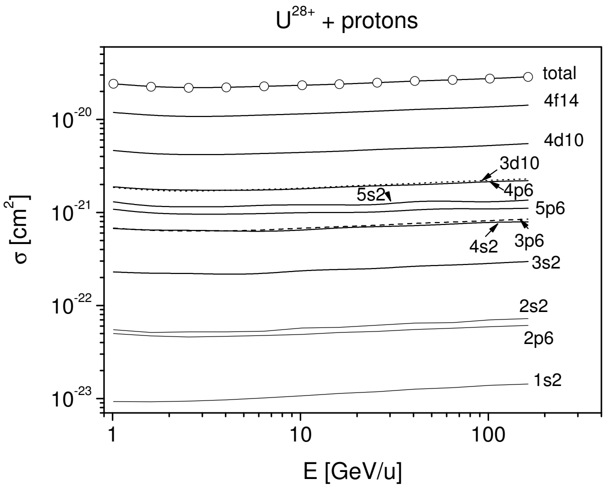

FIG. 1: Calculated ionization cross sections of $U^{28+}(1s^2...4f^{14}5s^25p^6)$ ions by protons: the LOSS-R - code [16]. Contribution of ionization from different subshells of U^{28+} are shown together with the total cross section.

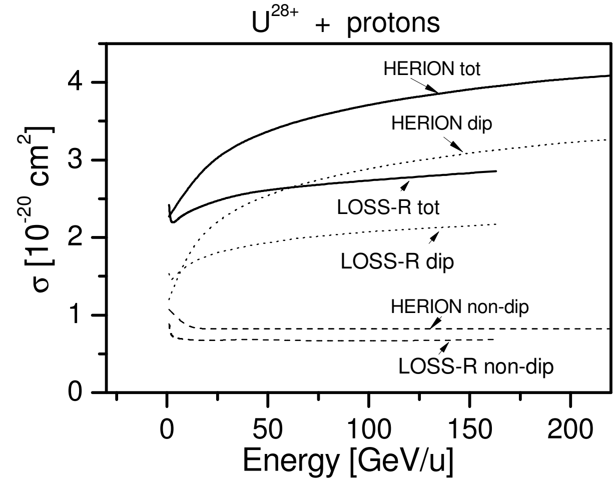

FIG. 2: Relativistic dipole, non-dipole and total ionization cross sections, i.e. summed over all nl shells, of U^{28+} by proton impact calculated by the HERION and LOSS-R codes (indicated): dashed curves - the non-dipole parts, dotted curves - the dipole parts, and solid curves - the total cross sections.

III. NUMERICAL CALCULATIONS

Calculated partial (on projectile electron subshells nl) and total ionization cross sections of U^{28+} ions by protons at energies E = 1 - 100 GeV/u are shown in Fig. 1. Calculations were performed by the LOSS-R code including dipole and non-dipole parts of the ionization cross sections and using the non-relativistic wave functions. As seen from the figure, the main contribution to the total cross section is given by electron ionization from $3d^{10}, 4p^6, 4d^{10}$,..., shells which can be described by the non-relativistic wave functions

A comparison of relativistic ionization cross sections of U^{28+} ions by proton impact calculated by two different codes, LOSS-R and HERION, is shown in Fig. 2 where the contributions from dipole-, non-dipole parts are shown together with the total (dipole + non-dipole) cross sections. In the LOSS-R code, the dipole part of the cross sections corresponds to electron transitions into the continuum with the orbital angular momentum quantum numbers $\lambda = l \pm 1$ where l is the angular momentum of the projectile-electron shell. As seen from the figure, the non-dipole parts calculated by the codes agree within 30 % meanwhile the dipole parts and the total cross sections agree only within a factor of 2. Most probably, this discrepancy is related to two reasons: first, the use of different wave functions in the codes, i.e., relativistic wave functions in HERION code and and non-relativistic ones in the LOSS-R code. And second, in the HERION code dipole ionization cross sections are calculated on the basis of photoionization cross sections; the latter are much higher than those calculated in the usual non-relativistic approximation because of the presence of the so-called giant resonances occurring due to configuration interaction of the final states (see [22] for details).

We note that the dipole part of ionization cross section involves about 60-70 % of the total cross section while the relativistic non-dipole part has a weak dependence on energy and, therefore, the dipole part has practically the same shape as the total cross section.

Relativistic ionization cross sections of $Au^{78+}(1s)$ ions in collisions with carbon are displayed in Fig. 3 where experimental data are given by symbols and theoretical calculations by curves. The non-relativistic result (LOSS) shows a Born maximum followed by a decrease of the cross section. The relativistic result (LOSS-R) has a local minimum around 1 GeV/u energy and increases logarithmically with energy. The results obtained with the HERION code have a little better agreement with experiment at $E > 200$ MeV/u than those by the LOSS-R code. In the calculations, the effective charge of the target $Z_T = Z^2 + N = 42$ was used while in the LOSS-R code the Z_T value is found in the q-representation with account of all subshells of the target (see eq. 27 and Ref. [4] for details). The lower curve is the recent result [15] with relativistic electron description.

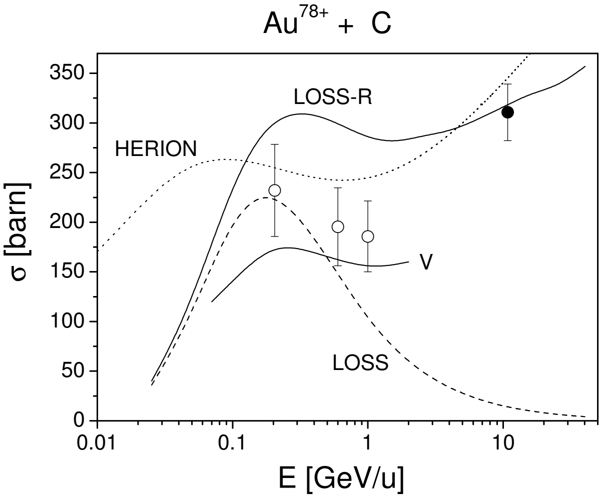

FIG. 3: Ionization cross sections of H-like $Au^{78+}(1s)$ ions by carbon atoms. Experiment: open circles - [12], [23] solid circle - [24]. Theory: LOSS - non-relativistic LOSS code [4], LOSS-R - relativistic LOSS-R code [16], HERION - HERION code [17] with effective target charge $Z_T^2 = Z^2 + N = 42$, V - calculations by Voitkiv [15] with relativistic electron description.

IV. NON-RELATIVISTIC LIMIT OF α-MATRIX ELEMENT

Now we consider the non-relativistic limit of the matrix-element G given by eq. (3):

$$G(q) =< f|\alpha_x exp(iqz)|i > .$$

The operator $J = \alpha_x \exp{(iqz)}$ is an odd one and connects the large and small components of the Dirac wave function. It gives zero if one only uses the large components. The non-relativistic limit of $G(q)$ is given in [25] in the form:

$$J = \frac{1}{2m}(\alpha_x exp(iqz)\rho_1(\vec{\sigma}\cdot\vec{p}) + (\vec{\sigma}\cdot\vec{p})\rho_1\alpha_x \exp{(iqz)}), \quad (9)$$

where $\vec{p} = \vec{e}_z q$. This operator acts only on the large component of the Dirac wave function. We use the relations $\alpha_x\rho_1 = \sigma_x$ and $\rho_1\alpha_x = \sigma_x$, (see [25], p. 891) to obtain

$$J = \frac{1}{2mc}(\sigma_x \exp{(iqz)}(\vec{\sigma}\cdot\vec{p}) + (\vec{\sigma}\cdot\vec{p})\sigma_x \exp{(iqz)}). \quad (10)$$

Using the identity $(\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B}) = (\vec{A}\cdot\vec{B}) + i\vec{\sigma}\cdot(\vec{A}\times\vec{B})$ (see e.g. eq. XIII.83 of [25]) with $\vec{A} = \vec{e}_x; \vec{B} = \vec{p}$ and with $\vec{B} = \vec{e}_x; \vec{A} = \vec{p}$ we find

$$J = \frac{1}{2m}(\exp{(iqz)}p_x + p_x \exp{(iqz)} + \mathrm{spin-flip\,terms}). \quad (11)$$

The spin-flip terms are given by

$$\exp{(iqz)}(\vec{p}\times\vec{\sigma})_x - (\vec{p}\times\vec{\sigma})_x \exp{(iqz)} \quad (12)$$

In the following, we neglect the spin-flip terms because they are small in our case, see also [5]). So the non-relativistic limit of the odd operator J is

$$J = \frac{1}{2m}(\exp{(iqz)}p_x + p_x \exp{(iqz)}. \quad (13)$$

This result can be also obtained directly using the electromagnetic-current approach in the Schrödinger theory (see, e.g., [26], Chapter 82a).

The spin-flip terms appear in the Pauli approximation, which can be obtained from the Dirac equation. The matrix element $G(q)$ becomes

$$G(q) = \frac{-i\hbar}{mc} < f|\exp(iqz)\frac{\partial}{\partial x}|i > . \quad (14)$$

Here $p_x = -i\hbar\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial x}e^{iqz} = 0$.

The derivative $\frac{\partial}{\partial z}$ is easier to calculate in spherical coordinates rather than $\frac{\partial}{\partial x}$, so we rotate the coordinate system by $\pi/2$ around the y-axis. This changes $x \to z$ and $z \to -x$. So we have

$$G(q) = \frac{-i\hbar}{mc} < f|\exp{(-iqx)}\frac{\partial}{\partial z}|i > . \quad (15)$$

Actually we only need the absolute square of the function G, summed over spins and integrated over the angle of the outgoing electron. This matrix element is calculated according to the rules of angular momentum algebra (see e.g., [27]). The bound state wave function $|i>$ is presented in the form $|i>= f_{l_i}(r)Y_{l_i m_i}(\hat{r})$, i.e. with separated angular and radial parts.

The exponential factor is expanded into partial waves in the usual way:

$$\exp{(-iqx)} = 4\pi\sum_{lm} i^{+l} j_l(qr) Y_{lm}(\hat{r}) Y^*_{lm}(\hat{x}) \quad (16)$$

The radial wave function of the bound and continuum states satisfy the normalization conditions:

$$\int_0^\infty g_{l_i}^2(r)dr = 1, \quad g_{l_f}(r) \approx \frac{1}{\sqrt{k}}\sin\left(kr + \frac{1}{k}\ln(2kr) + \eta\right), \quad k^2/2 = \epsilon, \quad (17)$$

where ϵ is the energy of ejected electron and η is the scattering phase shift.

According to [27] , the action of $\partial/\partial z$ on this wave function yields:

$$\partial\Psi/\partial z = \left(\frac{l+1}{\sqrt{(2l+1)(2l+3)}}Y_{l+1m} + \frac{l}{\sqrt{(2l-1)(2l+1)}}Y_{l-1m}\right)\partial f_l/\partial r$$
$$-(\frac{l(l+1)}{\sqrt{(2l+1)(2l+3)}}Y_{l+1m} - \frac{l(l-1)}{\sqrt{(2l-1)(2l+1)}}Y_{l-1m})f_l/r. \quad (18)$$

Thus, the matrix element is presented as a sum of angular and radial parts. We note that the present procedure is quite similar to that used for calculating the magnetic terms of the pionium breakup [28].

We define two types of radial matrix elements, a 'usual' one

$$R^B_{lf\lambda li}(q) \equiv \int_0^\infty drg_{lf}j_\lambda(qr)f_{li}, \quad (19)$$

and a 'new' one involving the derivative of the initial radial wave function:

$$R^d_{lf\lambda li}(q(q) \equiv \int_0^\infty drrg_{lf}j_\lambda(qr)\frac{df_{li}}{dr}. \quad (20)$$

The three-dimensional integration is, as usual, decomposed into a radial and angular parts. The angular integration can be done using eq. (4.6.3) in [27] and $Y^*_{lm} = (-1)^m Y_{l-m}$.

In the integration over the three spherical harmonics one obtains two types of terms: Ω_+ and Ω_- with

$$\Omega_\pm = \sqrt{\frac{(2l_f+1)(2\lambda+1)(2l_i\pm 1)}{4\pi}}\begin{pmatrix} l_f & \lambda & l_i\pm 1 \\ m_f & \mu & m_i \end{pmatrix}\begin{pmatrix} l_f & \lambda & l_i\pm 1 \\ 0 & 0 & 0 \\ . \end{pmatrix} \quad (21)$$

Collecting all the factors one obtains

$$G = \sum_{l_f m_f \lambda\mu} \frac{4\pi^2}{k}\, i^\lambda\, Y^*_{\lambda\mu}(\hat{x})Y^*_{l_f m_f}(\hat{k})$$
$$\times \left(\frac{l_i+1}{\sqrt{(2l_i+1)(2l_i+3)}}\Omega_+(R^d - l_i R) + \frac{l_i}{\sqrt{(2l_i-1)(2l_i+1)}}\Omega_-(R^d-(l_i-1)R)\right) \quad (22)$$

As was mentioned above, we need the function $|G(q)^2|$ integrated over Ω_k and summed over spins. The integration over Ω_k makes the sum over l_f and m_f incoherent, due to the orthogonality of the spherical harmonics. We assume that the states $j = l \pm 1/2$ are degenerate. Using the sum rules, the summation over m_i and m_f can be easily done:

$$\sum_{m_i m_f}\begin{pmatrix} l_f & \lambda & l_i\pm 1 \\ m_f & \mu & m_i \end{pmatrix}\begin{pmatrix} l_f & \lambda' & l_i\pm 1 \\ m_f & \mu' & m_i \end{pmatrix} = \delta_{\lambda,\lambda'}\delta_{\mu,\mu'}/(2\lambda+1) \quad (23)$$

The summation over μ can be also done using the completeness relation

$$\frac{4\pi}{2\lambda+1}\sum_\mu Y^*_{\lambda\mu}(\hat{x})Y_{\lambda\mu}(\hat{x}) = 1, \quad (24)$$

and one obtains the function $|G(q))|^2$ for given projectile quantum numbers n_i, l_i

$$|G(q)|^2 = \frac{2\hbar^2}{(mc)^2} \sum_{\lambda \mu l_f} |(l_i+1)u_+(R^d - l_i R) + l_i u_-(R^d + (l_i-1)R|^2 \quad (25)$$

The radial integrals R^B and R^d depend on q, l_f, λ, l_i according to eqs. (19) and (20), and $u_\pm$ is given by

$$u_\pm = \frac{\pi}{k} i^\lambda \sqrt{\frac{(2l_f+1)(2\lambda+1}{2l_i+1}} \begin{pmatrix} l_f & \lambda & l_i \pm 1 \\ 0 & 0 & 0 \\ . & & \end{pmatrix} \quad (26)$$

We note that $\lambda = 0$ corresponds to the dipole excitation, and a monopole contribution does not exist for the matrix element G but corresponds to the 'equivalent photon' contribution with the photon having spin 1. The monopole part is included to the the matrix-element F (see eqs. (1) and (2)).

Finally, for relativistic ionization cross section from the projectile electronic shell by a heavy target particle one can use eq. (1) but replacing the target effective charge Z_T by the q-dependent charge $Z_T(q)$ in the form:

$$Z_T^2(q) = \left(Z - \sum_{j=1}^{N_T} F_{jj}(q)^2\right)^2 + \left(N_T - \sum_{j=1}^{N_T} F_{jj}(q)^2\right), \quad F_{JJ}(q) =< j|\exp(i\mathbf{qr})|j >, \quad (27)$$

where Z and N_T denote the nuclear charge and the number of electrons of the target ($Z = N_T$ for neutral atoms and $Z = 1$, $N_T = 0$ for protons). The form of eq. 27 makes it possible to take into account the screening and anti-screening effects of all target electrons.

The function $F(q)$ in eq. (1) is the 'usual' Born matrix element which after separating angular and radial parts is written in the form:

$$|F(q)^2| = (2\lambda+1)(2l_f+1) \begin{pmatrix} l_i & l_f & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 |R^B(q)|^2, \quad (28)$$

where the Born integral $R^B(q)$ is given in eq. (19).

The function $G(q)$ describes the magnetic interactions between projectile ion and target atom and has the form:

$$\begin{aligned} |G(q)|^2 &= \frac{2}{c^2} \frac{(2\lambda+1)(2l_f+1)}{2l_i+1} \\ &\times \left| i^\lambda \begin{pmatrix} l_f & \lambda & l_i+1 \\ 0 & 0 & 0 \end{pmatrix} [(l_i+1)R^d(q) + l_i(l_i-1)R^B(q) + i^\lambda \begin{pmatrix} l_f & \lambda & l_i-1 \\ 0 & 0 & 0 \end{pmatrix} [l_i R^d(q) + l_i(l_i-1)R^B(q)] \right|^2 \end{aligned} \quad (29)$$

where the radial integral $R^d(q)$ is given by eq. (20).

V. CONCLUSION

Relativistic ionization of heavy ions colliding with atoms or ions is considered in the plane-wave Born approximation (PWBA). The ionization cross sections are presented in the momentum-transfer q-representation as a sum of two terms: the 'usual' Born approximation (matrix element of $i\mathbf{qr}$) and the relativistic term responsible for the magnetic interactions between colliding particles and expressed through the x-component α_x of the Dirac matrix vector $\vec{\alpha}$.

A simple limit of PWBA is the equivalent photon approximation (dipole approximation). Numerical calculations for the dipole and non-dipole parts of relativistic cross sections are presented for the p + U^{28+} and C+Au^{78+} collisions using the LOSS-R and HERION computer codes.

A new formula is obtained for the relativistic ionization cross section for an arbitrary nl shell of the projectile ion in the form of separated angular and radial parts. The radial part is expressed via an integral of the initial bound state wave function and the derivative of the final continuum wave function. In this way, new possibilies to investigate ionization processes including many electron atoms are opened.

VI. ACKNOWLEDGMENTS

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